MODELING COAL COMBUSTION IN FLUIDIZED BED REACTOR FOR ENERGY GENERATION[1]

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Abstract
The use of coal in combustion systems has been increased each day, because mainly depletion of petroleum and gas reserves, add the fact that coal is the most abundant world's fossil fuel. Fluidized bed combustion allows clean and efficient combustion of various solid fuels and models to describe the behavior of this equipment have already been proposed. This work aims to simulate the fluid dynamics of a fluidized bed combustor using the kinetic theory to consider the energy of particles fluctuation coupled with the kinetics of coal combustion in order to investigate the behavior of gas-solid phases. The present model consists of describing the phenomena that take place within an industrial scale reactor based on fluidized bed technology. The model is constructed based on transport equations of momentum, energy and chemical species of gas and pulverized phases. The PDE's are solved based on the finite volume method and appropriated boundary and initial conditions are selected to represent the industrial operational conditions. The rate equations of coal combustion are modeled by semi-empirical correlations found in the literature. Technological parameters such as productivity, combustibility and outlet gas composition and calorific values can be predicted by the model. The model is used to investigate bed instabilities such as bubbles formation and densification. Simulation results indicated that the model is in good agreement for simple system of isothermal fluidizations as demonstrated previously.
Key words: Fluidized bed; Multiphase flow; Mathematical modeling; Coal combustion.

MODELAMENTO DA COMBUSTÃO DE CARVÃO EM LEITO FLUIDIZADO PARA GERAÇÃO DE ENERGIA

Resumo
O uso do carvão em sistemas de combustão tem aumentado a cada dia, porque as reservas de gás e petróleo têm sofrido depleção, soma se a isto o fato do carvão ser o combustível fóssil mais abundante do mundo. Combustores de leito fluidizado permitem uma combustão eficiente e limpa de vários combustíveis sólidos e modelos para descrever o comportamento deste equipamento têm sido propostos. Este trabalho objetiva simular a fluidodinâmica de um combustor de leito fluidizado utilizando a teoria cinética para considerar a energia de flutuação das partículas acopladas à cinética da combustão de carvão com o intuito de investigar o comportamento das fases gás-sólido. O presente modelo consiste em descrever os fenômenos que ocorrem dentro de um reator em escala industrial baseado na tecnologia de leito fluidizado. O modelo é construído com base nas equações de transporte de momentum, energia e espécies químicas das fases gasosas e pulverizadas. As equações diferenciais parciais são resolvidas utilizando o método de volumes finitos com condições iniciais e de contorno apropriadas, que são selecionadas para representar as condições operacionais industriais. As taxas de combustão são modeladas a partir de correlações semi-empíricas encontradas na literatura. Parâmetros tecnológicos tais como produtividade, combustibilidade e composição do gás de saída são previstos pelo modelo. O modelo utilizado também investiga instabilidades no leito como a formação de bolhas e densificação. Os resultados da simulação mostram que o modelo está de acordo com sistemas simples de fluidização isotérmica.
Palavras-chave: Leito fluidizado; Escoamento multifásico; Modelamento matemático; Combustão de carvão.

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1 INTRODUCTION

The use of coal in combustion systems has been increased each day, because mainly depletion of petroleum and gas reserves, add the fact that coal is the most abundant world's fossil fuel.[1] Fluidized bed combustion allows clean and efficient combustion of various solid fuels and models to describe the behavior of this equipment have already been proposed.[2] These models try to explain the fluid dynamics behavior elucidating the particles movement in the system, trying to understand the emissions of pollutant gases objecting optimize CFB performances. The phases in this model are modeled using continuum mechanics principles where collection of particles is considered identical having a representative diameter and density. The solid phase momentum equation is modified by addiction of one term to account momentum exchange due to particle-particle collisions, this term including the kinetic theory model.[3] The granular temperature, Θ, is defined to represent the specific kinetic energy of velocity fluctuations or the translational fluctuation energy resulting from the particle velocity fluctuations.[4] In granular flow, particle velocity fluctuations about the mean are assumed to result in collisions between particles being swept along together by the mean flow. The granular particle temperature equation can be expressed in terms of production of fluctuations by shear, dissipation by kinetic and collisional heat flow, dissipation due to inelastic collisions, production due to fluid turbulence or due to collisions with molecules, and dissipation due to interaction with the fluid.[3] Many studies have shown the capability of the kinetic theory for modeling fluidized beds e.g. works of (Ding and Gidaspow, 1990), "Pain *et al*. (2001)".[5-6] Despite of the development of models to simulate fluidized beds have been achieved maturity, the results validation with experimental measurements must be done, mainly because some correlations used in the models are empirical or semi-empirical. This work considers a transient 3D model fluidized bed, where three phases are considered gas and two solid phases: one sand that is initial material in the bed and other coal. The fluid dynamics considering the motion three phases in a semi-industrial fluidized bed reactor is analyzed.

2 MATHEMATICAL MODEL

2.1 Transport Equation

The present model consists of describing the phenomena that happens inner of a semi-industrial fluidized bed reactor as a system of three phases that interact between it transferring mass, momentum and energy. The mathematical formulation follows hypothesis of the continuous media and as such can be formulated through transport equations. The phenomena of mass, momentum and energy exchange inner a fluidized bed reactor are represented by the general transport equation (equation 1). Where the index i represent the considered phase. The effective diffusion coefficient (Γ_ϕ) assumes different meanings and models in agreements of equation to be solved, for example if the momentum equation is the equation to be solved the effective diffusion coefficient assumes the dynamic viscosity. The source term (S_ϕ) represents generation or consumption of mass, momentum and energy. In the source term are considered for example the phenomena of interaction among phases, mechanics interactions resulting

in the coupling between the equations of conservation of mass, momentum and energy. The models of momentum and energy were obtained of literature and are detailed in another works for different studies.[4]

$$\frac{\partial \left(\varepsilon_i \rho_i \phi_i\right)}{\partial t} + div\ \left(\varepsilon_i U_i \phi_i\right) = div\ \left(\varepsilon_i \Gamma_{\phi_i} grad\ \ \phi_i\right) + S_{\phi_i} \tag{1}$$

The equation to consider the fluctuations energy of solid particles was introduced in the model and can be described by equation 2.[4]

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s \Theta_s\right) + grad\left(\varepsilon_s \rho_s \Theta_s \vec{v}_s\right)\right] = \left(-p_s \bar{I} + \bar{\tau}_s\right) \div grad\, \vec{v}_s + grad\left(k_{\Theta_s} \cdot grad\, \Theta_s\right) - \gamma_{\Theta_s} \tag{2}$$

Where, (Θ_s) is the granular temperature, (I) is the admensional stress tensor, ($\bar{\tau}_s$) is the stress tensor, p_s is the solid pressure, (γ_{Θ_s}) is the collision energy dissipation.

2.2 Computational Simulation

The simulation of fluidized bed consists to solve the governing equations of mass, momentum and energy in a semi-industrial fluidized bed reactor. The kinetic theory of granular flow is used to consider the conservation of solid fluctuation energy; it was used to closure of the solid stress terms.[4] The momentum exchange coefficients can be calculated by specifying drag functions. In this study the drag function used is the equation modified by Richardson and Zaki, which was modified to know the neighbors particles.[7] The drag function and drag coefficient are showed in the equations 3 and 4 respectively.

$$F_m = -C_{d_{g-s}}\left[\frac{3\,\varepsilon_s \rho_s}{4\,d_s \varphi_s}\right]\left|\vec{U}_g - \vec{U}_s\right|\left(\vec{U}_g - \vec{U}_s\right) \tag{3}$$

$$C_{d_{g-s}} = \left[\frac{24}{\mathrm{Re}_{g-s}}\left(1 + a\,\mathrm{Re}_{g-s}^{\,b}\right) + \frac{c}{1 + \frac{d}{\mathrm{Re}_{g-s}}}\right]\left(\frac{\varepsilon_g}{\varepsilon_g - \varepsilon_s}\right)^{-4,65} \tag{4}$$

The terms a, b, c and d in the drag coefficient equation are functions of shape factor of solid (φ).[7] To the set of differential equations represented by equation 1 must be imposed initial and boundaries conditions that represents the process to be simulated. The simulation parameters are in Table 1.

Table1. Fluidized bed reactor simulation parameters.

Description	Value	Comment
Particle density, ρ_p	2600 kg/m^3	sand
Gás density, ρ_g	1.225kg/m^3	Air
Particle diameter, d_p	2.5mm	Uniform distribution
Restitution coeficient, e_{ss}	0.90	Literature value
Initial fraction on the bed, ε_{s0}	0.60	Fixed value
Gas superficial velocity, U	0.1m/s	1.2*U_{mf}
Pressure of entry	1atm	Fixed value
Bed heigth	0.30m	Fixed value
Entry condition	Velocity	Gas velocity
Out conditions	Flow	Developed
Time steps	1s	Especified
Convergency criterion	10^{-6}	Especified

The energy sources that are results of chemical reactions, phase transformations and sensitive heat exchange due mass exchange, the energy source due convective heat is calculated by equation 5 and the heat exchange coefficient is calculated by Ranz Marshall equation 6.(7)

$$\dot{E}_i^j = h_{i-j} A_{i-j} \left[T_i - T_j \right] \tag{5}$$

$$h_{g-i} = \frac{K_g}{d_i} \left[2,0 + 0,6 \left(Re_{g-i} \right)^{0,5} \left(Pr_g \right)^{1/3} \right] \tag{6}$$

Chemical models - To simulate the evolution of chemical composition of injected coal, several chemical reactions were considered, which are summarized together with their kinetic models in Tables 2 to 6. For reaction kinetic models from literature were used. Carbon oxidation was assumed to occur in two ways. In the first one, the oxidation is partial, with generation of CO. In a second stage, CO is fully oxidized to CO_2. The solution loss and water gas shift reactions were considered as taking place at temperatures around 900ºC.

Table 2 – Combustion reactions of carbon

(1)	$C_{PC} + 1/2O_{2(g)} \rightarrow CO_{(g)}$
(2)	$C_{PC} + O_{2(g)} \rightarrow CO_{2(g)}$
$R_{(1)PC} = \frac{a}{1+a} R_{ave}$; $R_{(2)PC} = \frac{1}{1+a} R_{ave}$; $R_{ave} = \left(\frac{\varepsilon_g \rho_g \omega_{O_2(g)}}{M_{O_2}} \right) \left\{ \frac{d_i \varphi_i}{A_i D_{O_2,\omega_2}^{T_{ave}} Sh_i} + \frac{1}{\eta k_{ave}} \right\}^{-1}$	
$a = 2500 \exp\left(-\frac{12400}{1.987 T_i} \right)$; $k_{ave} = 7260 R T_g \exp\left(-\frac{17980}{T_{ave}} \right)$; $T_{ave} = \frac{T_g + T_i}{2}$; $A_i = \frac{6\varepsilon_i}{d_i \varphi_i}$ $\eta = \left[\frac{d_i}{6} \sqrt{\frac{k_{ave} \delta_i}{\zeta_i D_{O_2,N_2}^{T_{ave}}}} \right]^{-1} \left\{ \left[\tanh\left(\frac{d_i}{6} \sqrt{\frac{k_{ave} \delta_i}{\zeta_i D_{O_2,N_2}^{T_{ave}}}} \right) \right]^{-1} - \left[\frac{d_i}{2} \sqrt{\frac{k_{ave} \delta_i}{\zeta_i D_{O_2,N_2}^{T_{ave}}}} \right]^{-1} \right\}$; $\delta_{pc} = 1$; $\zeta_{pc} = 0.2$	

Table 3 – Kinetics model for Solution Loss reaction

(3)	$C_{PC} + CO_{2(g)} \rightarrow 2CO_{(g)}$
$R_{(3)} = \frac{\rho_g \omega_{Co_2(g)}}{M_{CO_2}} \left(\frac{1}{A_i k_{film,CO_2}} + \frac{1}{\eta k_{(3)}} \right)^{-1}$	
$k_{(3)_i} = \frac{k_1}{1 + k_2 P_{CO} + k_3 P_{CO_2}} \rho_i \varepsilon_i \omega_i 82{,}056 \times 10^{-3} T_g$; $k_1 = \frac{1}{60} \exp\left(19{,}875 - \frac{66350}{1{,}987 T_i} \right)$ $k_2 = \exp\left(-6{,}688 + \frac{21421}{1{,}987 T_i} \right)$; $k_3 = \exp\left(31{,}615 - \frac{88168}{1{,}987 T_i} \right)$; $k_{film,CO_2} = D_{CO_2,N_2}^{T_{ave}} \frac{Sh_i}{d_i \varphi_i}$ $P_{\omega_j} = \frac{82{,}056 \times 10^{-3} \rho_g T_g \omega_j}{M_{\omega_j}}$;(j=CO,CO2); $A_i = \frac{6\varepsilon_i}{d_i \varphi_i}$; $\eta = \left[\frac{d_i}{6} \sqrt{\frac{k_{10_i} \delta_i}{\zeta_i D_{O_2,N_2}^{T_{ave}}}} \right]^{-1} \left\{ \left[\tanh\left(\frac{d_i}{6} \sqrt{\frac{k_{10_i} \delta_i}{\zeta_i D_{O_2,N_2}^{T_{ave}}}} \right) \right]^{-1} - \left[\frac{d_i}{2} \sqrt{\frac{k_{10_i} \delta_i}{\zeta_i D_{O_2,N_2}^{T_{ave}}}} \right]^{-1} \right\}$; $T_{ave} = \frac{T_g + T_i}{2}$; $\delta_{pc} = 1$; $\zeta_{pc} = 0{,}2$	

Table 4 – Kinetics model for Water Gas Reaction

(4)	$C_{PC} + H_2O_{(g)} \rightarrow CO_{(g)} + H_{2(g)}$

$$R_{(4)} = \frac{\rho_g \omega_{H_2O(g)}}{M_{H_2O}} \left(\frac{1}{A_i k_{film,H_2O}} + \frac{1}{\eta k_{(4)}} \right)^{-1}$$

$$k_{(4)} = \frac{k_4}{1 + k_2 P_{CO} + k_3 P_{CO_2} + k_5 P_{H_2O}} \omega_{C_{(i)}} \rho_i \varepsilon_i 82{,}056 \times 10^{-3} T_g \; ; \; k_2 = 10{,}3 \frac{M_{H_2O}}{M_{CO}}$$

$$k_{film,H_2O} = D^{T_{ave}}_{H_2O,N_2} \frac{Sh_i}{d_i} \; ; Sh_i = 1{,}5 Re_g^{0{,}55} \; ; \; k_3 = \frac{M_{H_2O}}{M_{CO_2}} \exp\left(14{,}24 - \frac{18350}{T_i}\right)$$

$$A_i = \frac{6\varepsilon_i}{d_i \varphi_i} \; ; \; k_4 = \frac{1}{3600 M_C} \exp\left(22{,}35 - \frac{26320}{T_i}\right) ; \; k_5 = \exp\left(29{,}59 - \frac{36760}{T_i}\right) ;$$

$$P_{\omega_j} = \frac{82{,}056 \times 10^{-3} \rho_g T_g \omega_j}{M_{\omega_j}}$$

$$\eta = \left[\frac{d_i}{6} \sqrt{\frac{k_{10_i} \delta_i}{\zeta_i D^{T_{ave}}_{H_2O,N_2}}} \right]^{-1} \left\{ \left[\tanh\left(\frac{d_i}{6} \sqrt{\frac{k_{10_i} \delta_i}{\zeta_i D^{T_{ave}}_{H_2O,N_2}}} \right) \right]^{-1} - \left[\frac{d_i}{2} \sqrt{\frac{k_{10_i} \delta_i}{\zeta_i D^{T_{ave}}_{H_2O,N_2}}} \right]^{-1} \right\} ;$$

$$\delta_{pc} = 1 ; \zeta_{pc} = 0.2$$

Table 5 – Kinetics model for Water Shift reaction

(5)	$CO_{2(g)} + H_{2(g)} \leftrightarrow CO_{(g)} + H_2O_{(g)}$

$$R_{(5)} = \frac{1000}{(101325)^2} \varepsilon_s (f_{PC}) k_{(5)} \left(P_{CO} P_{H_2O} - \frac{P_{co} P_{H_2O}}{k_{(5)}} \right)$$

$$P_{\omega_j} = \frac{82{,}056 \times 10^{-3} \rho_g T_g \omega_j}{M_{\omega_j}} \; ; \; k_{(5)} = \exp\left(-3{,}5414 + \frac{3863{,}7}{T_i}\right) ; \; k_1 = 93{,}3 \exp\left(\frac{-7{,}32}{8{,}3146 \times 10^{-3} T_g}\right)$$

$$k_{(5)} = \alpha k_1 + (1 - \alpha) k_3 \; , \; \left(P_{CO} P_{H_2O} - \frac{P_{CO_2} P_{H_2}}{K_{12}} \right) \geq 0 \; ; \; k_2 = 136 \exp\left(\frac{-7{,}75}{8{,}3146 \times 10^{-3} T_g}\right)$$

$$k_{(5)} = [\alpha k_2 + (1 - \alpha) k_4 \,] k_{(5)} \; ,$$

$$\left(P_{CO} P_{H_2O} - \frac{P_{CO_2} P_{H_2}}{K_{12}} \right) < 0 \; ; \; k_3 = 1{,}83 \times 10^{-5} \exp\left(\frac{7{,}84 \times 10^{-3}}{8{,}3146 \times 10^{-3} T_g}\right) ;$$

$$k_4 = 8{,}83 \times 10^{-2} \exp\left(\frac{4{,}56}{8.{,}146 \times 10^{-3} T_g}\right)$$

Table 6 - Kinetics model for volatile combustion

(6)	$\text{Volatiles}_{(pc)} + \alpha_1 O_{2(g)} \rightarrow \alpha_2 CO_{2(g)} + \alpha_3 H_2O_{(g)} + \alpha_4 N_{2(g)}$
$R_{(6)} = 23{,}6\left(\frac{\mu_g \varepsilon_t}{\rho_g k_t}\right)^{1/4}\left(\frac{\varepsilon_t}{k_t}\right)\min\left(\varepsilon_{pc}\rho_{pc}\omega_{MVPC}, \varepsilon_g \omega_{O_2}\frac{M_{MV}}{\alpha_1 M_{O_2}}\right)$	
(7)	$\text{Volatiles}_{(pc)} + \alpha_5 CO_{2(g)} \rightarrow \alpha_6 CO_{(g)} + \alpha_7 H_{2(g)} + \alpha_8 N_{2(g)}$
$R_{(7)} = 23{,}6\left(\frac{\mu_g \varepsilon_t}{\rho_g k_t}\right)^{1/4}\left(\frac{\varepsilon_t}{k_t}\right)\min\left(\varepsilon_{pc}\rho_{pc}\omega_{MVPC}, \varepsilon_g \omega_{CO_2}\frac{M_{MV}}{\alpha_5 MC_{O_2}}\right);$ $k_t = \left(0.03\left\|\vec{U}_g\right\|\right)^2; \varepsilon_t = \frac{k_t^{0.5}}{0.01}$	

3 Results and Discussion

This section presents some previous results of combustion model reactions obtained with the developed fluidized combustor model. The results are obtained after the preheating of reactor until initial bed particles reaching 450º C, in this moment the coal feeding starts and the combustion system is activated. The Figure 1 shows schematic reactor figure representing the geometry. Figure 2 shows the mesh obtained by discretization of PDE's equation using the finite volume method. Figure 3 shows the behavior of coal in the bed, where can be sight the accumulation in the bottom. This fact represents a solid hold-up meaning that particles not burned yet are deposited in some regions of fluidized bed. Figure 4 shows the concentration of oxygen into the fluidized bed that concentrate more in the bottom of reactor because the gas enters by the bottom, in superior parts of reactor the concentration decreases because part is consumed by coal combustion process. Figure 5 shows the concentration of CO in the inferior corner where coal is accumulated in other parts the concentration is distributed into the reactor. Figure 6 shows the CO_2 concentration into the bed this is minor in the region where coal is accumulated, because the partial combustion of carbon presents in the model reaction rate larger than total combustion. Figure 7 shows the concentration of gases curves into the reactor against the time this graph shows the variation of gases with combustion time. The concentration of O_2 decreases with time because this gas is consumed by reactions; on the other hand the gases that are products of reactions like CO, CO_2 and H_2O increase their concentrations with time evolution.

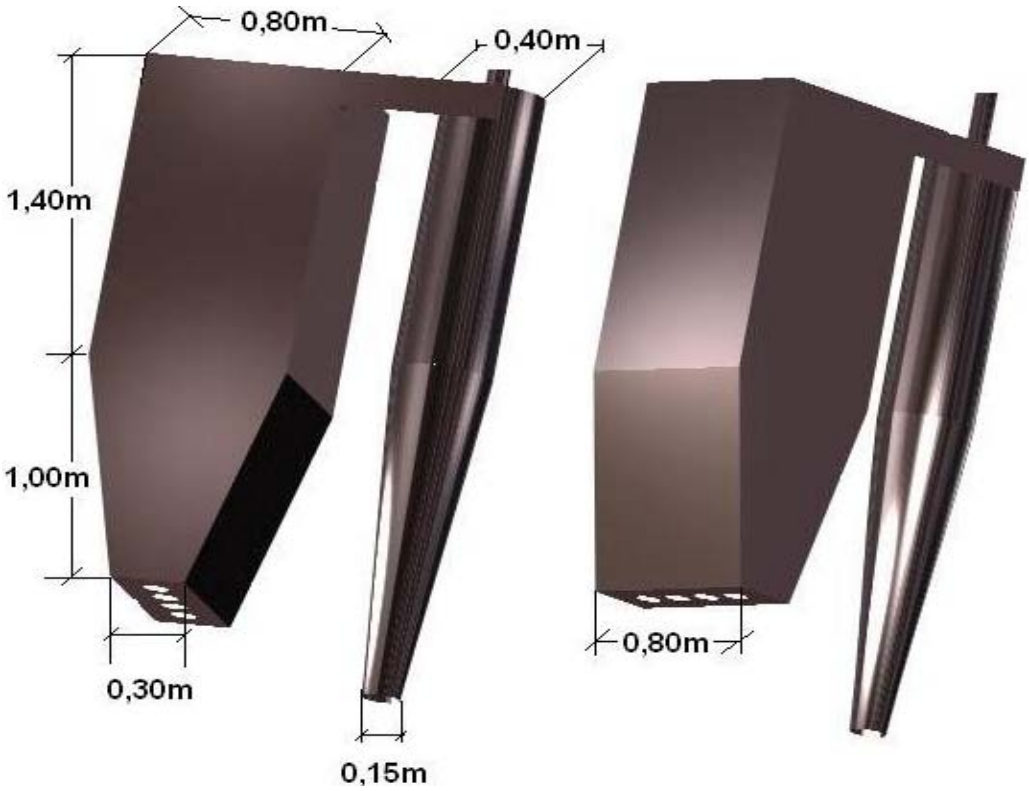

Figure 1. Schematic figure of fluidized bed reactor.

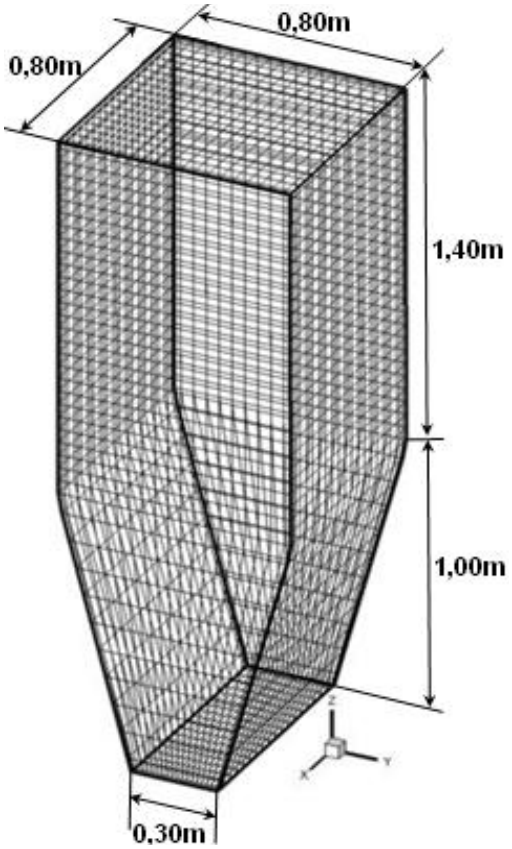

Figure 2. Mesh generated by volume finite method.

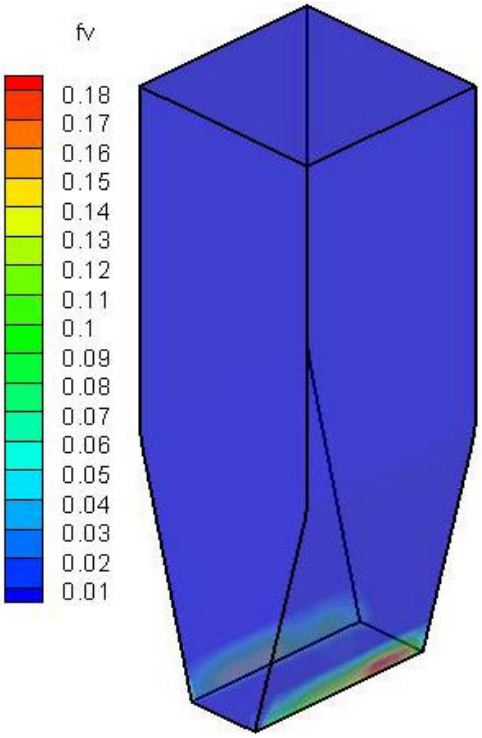

Figure 3. Solids hold up in fluidized bed.

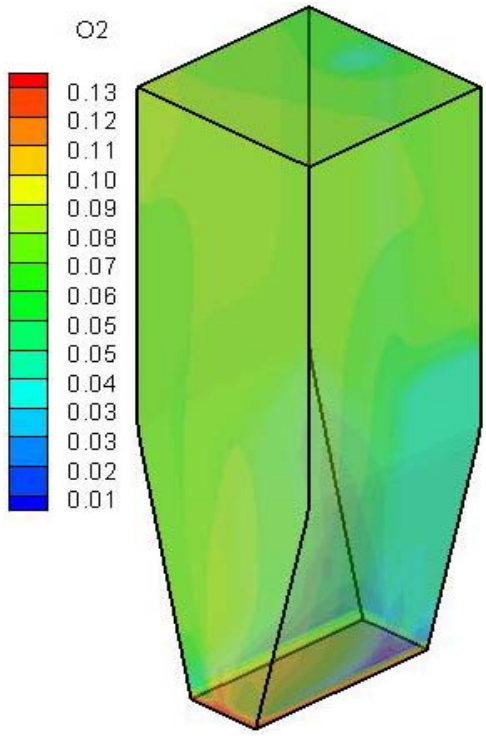

Figure 4. Concentration of O_2 in the bed.

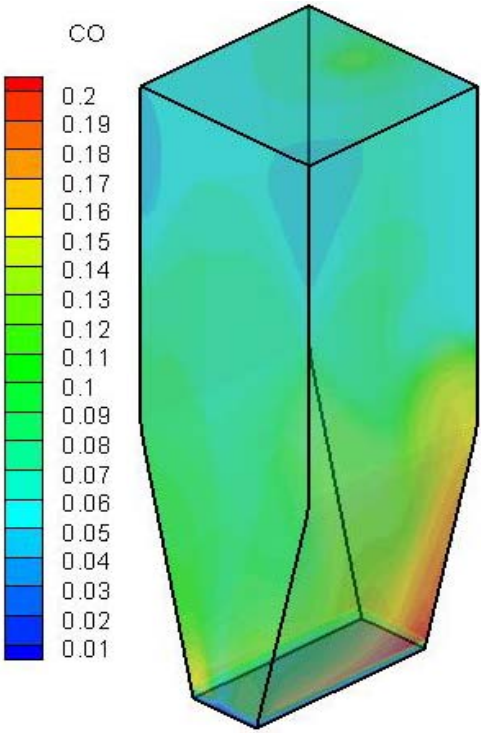

Figure 5. Concentration of CO in the bed

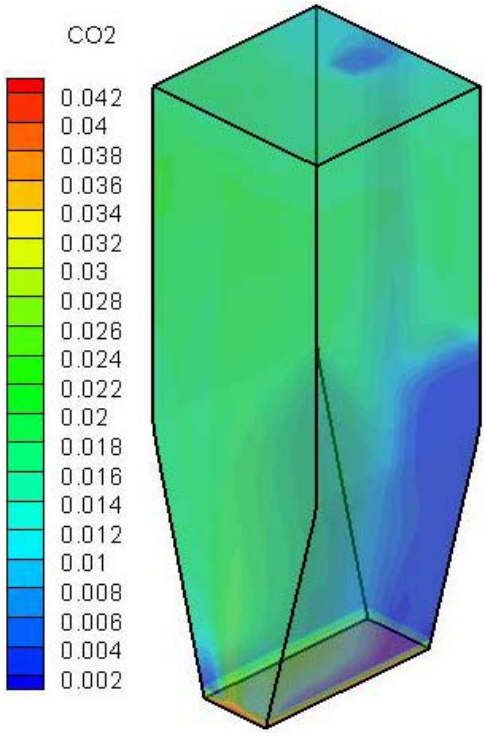

Figure 6. Concentration of CO_2 in the bed.

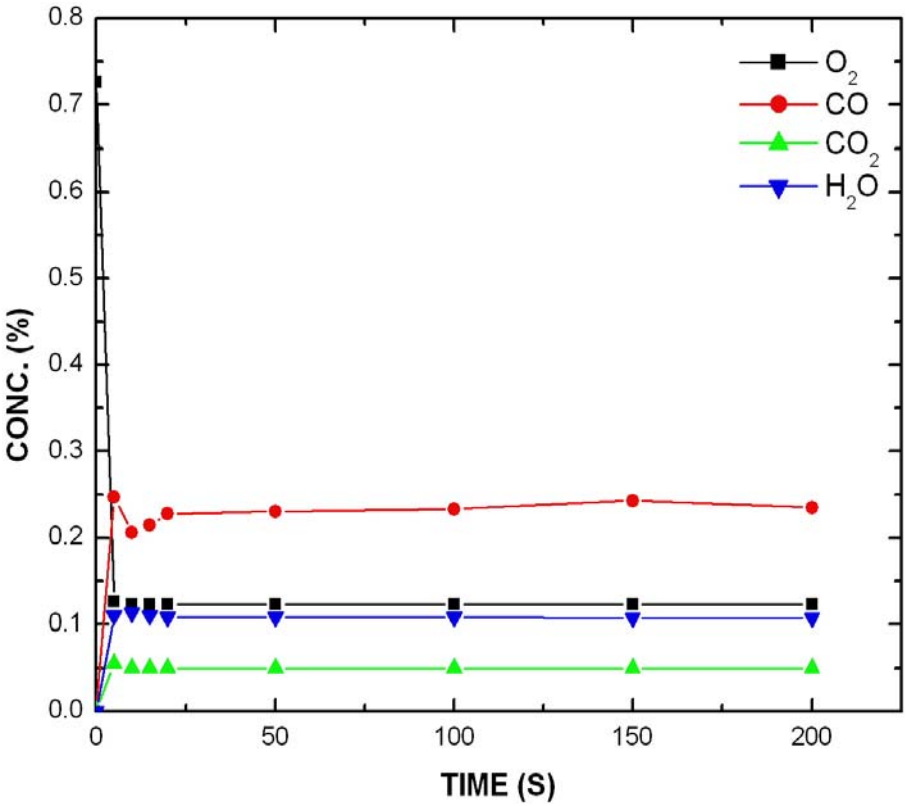

Figure 7. Gases concentration curves in the reactor.

4 CONCLUSIONS

A mathematical model for simulating pulverized coal combustion in fluidized bed reactor has been developed. The model is based on a three phase multi-component system which interacts with one another exchanging momentum, mass and energy. As presented results showed the developed model showed compatibles results with literature. The fluid dynamic behavior and reaction kinetics are in good agreement with previous results consulting to development the model, although some adjusts needs to be done for better results and model accuracy and efficiency. The needs adjusts to be done for representing better the fluidized bed phenomena mainly in the reactions rate where the presented results not representing the real behavior of gases in the system yet. These results are preliminaries and as kinetic models were take out literature they needs adjust to represent better the combustion gases behavior.

Aknowlegments

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REFERENCES

1 BORAH, D., *Electron-Transfer-Induced desufurization of organic sulfur from sub-bituminous coal*, Energy & Fuels, vol. 18, p. 1463-1471, 2004.

2 DESROCHES-DUCARNE, E. et al., *Modelling of gaseous pollutants emissions in circulating fluidized bed combustion of municipal refuse,* Fuel, vol. 77, Nº. 13, p. 1399-1410, 1998.

3 GIDASPOW, D., 1994, *Multiphase flow and fluidization: Continuum and kinetic theory descriptions*, Academic press, San Diego.

4 TAGHIPOUR, F., ELLIS. N., WONG, C., *Experimental and computational study of gas-solid fluidized bed hydrodynamics*, Chemical Engineering Science, vol. 60, p. 6857-6867, 2005.

5 DING, J., GIDASPOW, D., *A bubbling fluidization model using kinetic theory of granular flow,* AIChEJournal, vol.36, Nº 4, p. 523-538, April 1990.

6 PAIN, C. C., et al., *A study of bubbling and slugging fluidised beds using the two-fluid granular temperature model,* International journal of multiphase flow, vol. 27, p. 527-551, 2001.

7 CASTRO, J.A*., A multi-dimensional transient mathematical model of blast-furnace based on mult-fluid model*, Institute for advanced material processing, Tohuku University, Japan, Doctored thesis, 2000.